Effect of pre-anneal chemistry on the growth and properties of epitaxial MoS_2 on sapphire

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Two-dimensional transition metal dichalcogenides (TMDs) such as MoS_2 hold great promise in a wide variety of electronic and optoelectronic applications. Large, wafer-scale coalesced TMD films can be grown epitaxially on sapphire using different deposition methods, including metal organic chemical vapor deposition (MOCVD). Prior studies have suggested that chalcogen atoms help passivate dangling bonds on the sapphire surface, thus enabling quasi- van der Waals epitaxy [1,2]. However, the exact impact of chalcogen passivation on the growth on TMD films is not well-understood.

In this work, we study the effect of pre-annealing c-plane sapphire under H_2 vs a mixture of H_2 and H_2S, on the nucleation, growth, and properties of MOCVD-grown epitaxial MoS_2. When pre-annealed under pure H_2, the MoS_2 nucleates rapidly and randomly on the sapphire, quickly reaching saturation. These domains then laterally grow outwards, merging to form a coalesced film. In contrast, when the sapphire is pre-treated with a mixture of H_2 and H_2S, the MoS_2 preferentially nucleates along the sapphire step edges, likely due to preferential sulfur passivation of dangling bonds on the sapphire terraces versus steps. Due to the greater separation between the MoS_2 domains across a step terrace than between those along the same step edge, a non-regular, network-like growth occurs, resulting in elongated and aligned voids that close upon coalescence.

Coalesced films were grown after different pre-anneal conditions and characterized to determine the effect of the pre-anneal on the final film properties. In-plane XRD measurements show that MoS_2 grown on H_2 pre-annealed sapphire has greater compressive stress than when the film is grown in H_2/H_2S pre-anneal substrates. This difference in strain was also observed using Raman and photoluminescence spectroscopy and is likely due to the pinning of MoS_2, preventing film relaxation. Additionally, the H_2 pre-annealed sample displayed a $[11\bar{2}0]MoS_{2(0001)}$ // $[11\bar{2}0]$a-$Al_2O_{3(0001)}$ epitaxial relationship, while the epitaxy for the H_2/H_2S pre-annealed sample is rotated by 30° to $[11\bar{2}0]MoS_{2(0001)}$ // $[2\bar{1}\bar{1}0]$a-$Al_2O_{3(0001)}$. The impact of the pre-anneals on the grain structure and electrical and optical properties of the MoS_2 layers will be presented.

[1] Lin YC et al. Realizing Large-Scale, Electronic-Grade Two-Dimensional Semiconductors. ACS Nano. 2018;12(2): 965–975

[2] Xiang Y et al. Monolayer MoS2 on sapphire: an azimuthal reflection high-energy electron diffraction Perspective. 2D Mater. 2021; 8(2): 025003.